

Acta Cryst. (1973). **B29**, 1554

Criteria for hydrogen bonding. II. A hydrogen bond in the edge of a coordination polyhedron around a cation.

Erratum. By WERNER H. BAUR, *Department of Geological Sciences, University of Illinois at Chicago, Chicago, Illinois 60680, U.S.A.*

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The bond length Cs-O(4) given in Table 1 in *Acta Cryst.* (1973), **B29**, 139 should be 3.515 Å.

Because of a misprint the value of the bond length Cs-O(4) in Table 1 (Baur, 1973) reads as 3.315 Å. The correct value of Cs-O(4) is 3.515 Å. Therefore the statement (Baur, 1973) 'that the distance Cs-O(4) to the acceptor atom of the hydrogen bond is the largest of the distances considered to belong to the coordination polyhedron around the Cs-atom' is correct after all, even though it is not apparent from Table 1 as

it was printed. Since atom O(4) is the acceptor atom of the hydrogen bond located in the edge of the coordination polyhedron around the Cs atom it is significant that Cs-O(4) is a long bond.

Reference

BAUR, W. H. (1973). *Acta Cryst.* **B29**, 139-140.

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Orientation relation in the transformation of the NaCl-related to the CsCl-related structure in rubidium nitrate.

By A. J. IVERSEN and S. W. KENNEDY, *Physical and Inorganic Chemistry Department, University of Adelaide, Adelaide 5001, Australia*

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The structure transformation RbNO_3 I (NaCl-like) \rightarrow II \rightarrow III (CsCl-like) proceeds topotaxically, with an orientation relation in which $[100]_{\text{I}} \parallel [100]_{\text{III}}$. Despite the presence of the complex ion the relation is similar to one of the relations observed in the transformations NaCl-type \rightleftharpoons CsCl-type in NH_4Br .

It has already been shown that the forward and reverse transformations CsCl-type (simple cubic) \rightleftharpoons NaCl-type (f.c.c.) are topotaxic in that definite orientation relations result, and there is evidence that at least on supercooling the mechanism is martensitic (Fraser & Kennedy, 1972; Kennedy, Patterson, Chaplin & Mackay, 1973). It has not been known how far crystal-chemical relations can result in topotaxy when in addition to a large lattice deformation, the planar complex ions such as NO_3^- , CO_3^{2-} , must tilt during the transformation. Rubidium nitrate affords a test of this. In rubidium nitrate an NaCl-like f.c.c. phase (I) (having randomized orientations of anions) (Kennedy, 1970a; Strømme, 1971) is linked to a CsCl-like cubic phase III (Korhonen, 1951) through a phase II which is stable between 219 and 284°C. Phase II is commonly considered to be rhombohedral, calcite-like (*e.g.* Salhotra, Subbarao & Venkateswarlu, 1968) but tetragonal symmetry has also been suggested (Brown & McClaren, 1962). The primitive cubic cell of phase III is a sub-cell, the plane of the anion being differently oriented in neighbouring sub-cells. The volume change III \rightarrow I of 16% is the same as in CsCl and NH_4Br , but $\Delta V_{\text{III} \rightarrow \text{II}}/V_{\text{III}} = 0.1$ and $\Delta V_{\text{II} \rightleftharpoons \text{I}}$ is small, the remainder being accounted for by thermal expansion of II (Salhotra, Subbarao & Venkateswarlu, 1968). Because of the disruption previously observed at the transformation III \rightarrow II in needle-like crystals it has been considered that in practice the large structure and volume-change do not permit topotaxy (Brown & McClaren, 1962). Topotaxy in the transformation II \rightarrow I (Kennedy, 1966), and in I \rightarrow II with fine twinning (Kennedy, 1970a) has already been reported. The present work shows that a definite orientation

relation is also maintained between the NaCl-like phase I and the CsCl-like phase III during the transformations I \rightarrow II \rightarrow III.

Single crystals of RbNO_3 I were grown from the melt at 310°C on glass cover-slips on a flat heater carried on the goniometer head of an X-ray camera, which itself carried a detachable polarising microscope. Form I was oriented, and the orientation of III determined, by precession and front-reflexion Laue photographs, the X-rays being transmitted through the glass.

The resulting finely twinned specimens of phase II detwinned after 15 min, giving up to six reproducible orientations. When such detwinned specimens were maintained slightly below 219°C fine platelets of phase III appeared in three orientations within each single block of phase II (Kennedy, 1970b). The traces of the platelets were parallel to the traces of the twin-plane of the calcite-like structure. The platelets grew first into blocks and then into an irregular shape. Fine remnants of phase II trapped between adjacent regions of phase III could be supercooled to 164°C. Only one type of orientation was found both in individual specimens, and in repeated experiments:

$$\begin{aligned} (001)_{\text{I}} \parallel (011)_{\text{III}} \\ [100]_{\text{I}} \parallel [100]_{\text{III}} \end{aligned}$$

This however is a mean orientation. The reflexions were split into several components which corresponded to individual orientations differing from this mean by up to 5°. The splitting of the reflexions is probably due to variants of an irrational relation. This result is the converse of relation C of Kennedy, Patterson, Chaplin & Mackay (1973)

for $\text{NH}_4\text{Br II} \rightarrow \text{I}$ and close to relation *C* of Fraser & Kennedy (1972) for $\text{NH}_4\text{Br I} \rightarrow \text{II}$, and is probably a secondary orientation in CsCl (Chatterji, Mackay & Jeffery, 1970). The commonly accepted lattice correspondence relates f.c.c. and primitive cubic (or rhombohedral) through the primitive rhombohedron of the f.c.c. lattice (Shoji, 1931) the lattice transformation being effected by a pure strain the principal axis of which is the common [111] direction. This is only one component of the total deformations that would also accommodate the structures, but the additional rotation that would produce the present relation is unexpectedly large. In fact the relation corresponds to the Bain strain (principal axis $[100]_I$), which would have to be combined with shears to produce the structure of III. Whilst the twinning in the transformation $\text{I} \rightarrow \text{II}$ was consistent with a martensitic mechanism, detailed discussion of the mechanism of $\text{II} \rightarrow \text{III}$ especially awaits further investigations.

The results already obtained nevertheless imply topotaxy not only between the NaCl-like and CsCl-like phases, but also between the RbNO_3 II and low- RbNO_3 structures. They support the view that a large structure change is consistent with topotaxy in chemical compounds; and they imply that though a particular variation may be favoured, the transformations of compounds of complex ions can fol-

low the same geometry that applies to compounds of simple or near-spherical ions.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

New Co-editor of *Acta Crystallographica*

The Executive Committee of the International Union of Crystallography has approved the appointment of Profes-

sor G. A. Jeffrey as a Co-editor of *Acta Crystallographica*. Professor Jeffrey will take up this work on 1 August 1973. His address is given in the list of Co-editors on the inner front cover of this issue.

Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

BIDICS (Bond index to the determination of inorganic crystal structures) - 1969, 2nd ed. By I. D. BROWN and C. P. WEISS; pp. 108,
BIDICS - 1970, 2nd ed. By I. D. BROWN and C. P. WEISS; pp. 113,
BIDICS - 1971. By I. D. BROWN, C. P. WEISS and K. K. WU, pp. 126. Institute for Materials Research, McMaster University, 1972. Price (1969 and 1970) Canadian \$3.00, (1971), Canadian \$7.50 (paperback).

'BIDICS' is an acronym for Bond Index to the Determinations of Inorganic Crystal Structures. The aim is to provide a rapid and cheap service to enable anyone, not necessarily a qualified crystallographer, to discover the reference to a crystal structure containing an interatomic distance of in-

terest. Included are all crystal structures, except those of purely organic compounds, published in about 35 journals during the year in the title.

Each volume is in two parts, the first being a list of the shortest interatomic distances of each type in the compounds or minerals with chemical formulae and abbreviated references which lead to the second part, the bibliography. Entry is only through interatomic distances, *i.e.* there is no author index. BIDICS is designed to answer the question 'Where were Na–O distances reported in 1969?' In this it is successful. It can also be used to answer the question 'Was the structure of $\text{NaHSO}_2\text{HCHO}\cdot 2\text{H}_2\text{O}$ determined in 1970?'

Its most serious limitation is the small number of fairly common journals covered, so it is not comprehensive. A minor one is the use of line-printer output with its restricted